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Notes on D-optimal designs

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Abstract

The purpose of this paper is to exhibit new infinite families of D-optimal $(0,1)$-matrices. We show that Hadamard designs lead to D-optimal matrices of size (j, mj) and $(j-1, mj)$, for certain integers $j \equiv 3 \pmod 4$ and all positive integers m. For j a power of a prime and $j \equiv 1 \pmod 4$, supplementary difference sets lead to D-optimal matrices of size $(j, 2mj)$ and $(j-1, 2mj)$, for all positive integers m. We also show that for a given j and d sufficiently large, about half of the entries in each column of a D-optimal matrix are ones. This leads to a new relationship between D-optimality for $(0,1)$-matrices and for (± 1)-matrices. Known results about D-optimal (± 1)-matrices are then used to obtain new D-optimal $(0,1)$-matrices.

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1. Introduction

Let $M_{j,d}(0,1)$ be the set of all $j \times d$ $(0,1)$-matrices. The problem of finding the maximum value of $\det AA^{\mathrm{T}}$ for $A \in M_{j,d}(0,1)$ has received considerable attention over the past several decades primarily for its significance in statistical design theory. In 1944, Hotelling [1] initiated the use of Hadamard matrices to analyze the problem of estimating the weights of j objects with d weighings. Any selection of the j objects can be placed on a scale for a given weighing.

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The information for all d selections of objects can be coded into a $j \times d$ *design matrix* $A \in M_{j,d}(0,1)$ in which the ones in column c correspond to the objects selected for weighing $c = 1, \ldots, d$. Some design matrices are better than others in the sense that the confidence regions in $\mathbb{R}^j$ for the j-tuple of weights are smaller. Indeed under certain normality assumptions on the distribution of weighing errors, design matrices A for which det AA^{T} is maximal produce the smallest confidence regions [2]. These design matrices are called *D-optimal matrices*.

There is also a geometric interpretation of det AA^{T}. The volume of the j-simplex in $\mathbb{R}^d$ generated by the j rows of A and the origin is $(1/j!)(\det AA^{\mathrm{T}})^{1/2}$. Thus the problem of finding a largest j-simplex in the d-dimensional unit cube is equivalent to finding a matrix $A \in M_{j,d}(0,1)$ for which det AA^{T} is maximum.

D-optimal matrices are known for $j = 2, 3$ and all values of $d \geqslant j$ [3]. But for $j \geqslant 4$ the results are sporadic and incomplete. The purpose of this paper is to exhibit D-optimal matrices in $M_{j,d}(0,1)$ for infinite families of pairs (j, d). In Section 3 we show that Hadamard designs (which we describe later) lead to D-optimal matrices of size (j, mj) and $(j-1, mj)$ for certain integers $j \equiv 3 \pmod 4$ and all positive integers m. And for j a power of a prime and $j \equiv 1 \pmod 4$, supplementary difference sets lead to D-optimal matrices of size $(j, 2mj)$ and $(j-1, 2mj)$, for all positive integers m.

In Section 4 we show that for a given j and sufficiently large values of d, each D-optimal matrix of size (j, d) must have about one half of its entries in each column equal to 1. In particular, for $j = 2k-1$ odd and d sufficiently large, each D-optimal matrix of size (j, d) must have exactly k ones in each column. It is precisely this fact that is needed to establish a new relationship between D-optimality for $(0,1)$-matrices and for (± 1)-matrices. And since the theory of (± 1)-matrices is more developed, in Section 5 we are able to use some of the results for D-optimal (± 1)-matrices to obtain new D-optimal $(0,1)$-matrices.

In the following, I_j denotes the $j \times j$ identity matrix, $J_{j,d}$ denotes the $j \times d$ matrix all of whose entries are 1, and $J_j = J_{j,j}$. When the size of these matrices is clear from the context, we omit the subscripts. We use $m * A = [A, A, \ldots, A]$ to denote the matrix A concatenated m times. Following [3] we define

$$G(j,d) = \max\{\det AA^{\mathrm{T}}\colon A \in M_{j,d}(0,1)\}. \tag{1}$$

2. Regular D-optimal matrices

We begin this section with known upper bounds for det AA^{T} separated into two cases – j odd and j even. The inequality in Theorem 2.1 appears in [3], while [4] contains the result in Theorem 2.2 as well as an analysis for the cases of equality in both theorems.

Theorem 2.1 ([3]). *If $j = 2k - 1$ is odd and $A \in M_{j,d}(0,1)$, then*

$$\det AA^{\mathrm{T}} \leqslant (j+1)\left(\frac{(j+1)d}{4j}\right)^{j}. \tag{2}$$

Equality holds in Eq. (2) if and only if

1. $AA^{\mathrm{T}} = t(I+J)$, *for some integer t and either of the following conditions are met:*

2a. *each column of A contains exactly k ones*

or

2b. $t = (j+1)d/4j$.

Theorem 2.2 ([4]). *If $j = 2k$ is even and $A \in M_{j,d}(0,1)$, then*

$$\det AA^{\mathrm{T}} \leqslant (j+1)\left(\frac{(j+2)d}{4(j+1)}\right)^{j}. \tag{3}$$

Equality holds in Eq. (3) if and only if

1. $AA^{\mathrm{T}} = t(I+J)$, *for some integer t and either of the following conditions are met:*

2a. *each column of A contains either k or $k+1$ ones*

or

2b. $t = (j+2)d/4(j+1)$.

A D-optimal matrix A is a *regular* if it satisfies the conditions for equality in Theorem 2.1 or in Theorem 2.2. It is convenient to define a symbol $B(j,d)$ for the upper bounds in Theorems 2.1 and 2.2. For $j = 2k-1$ odd, define

$$B(j,d) = (j+1)\left(\frac{(j+1)d}{4j}\right)^{j} \tag{4}$$

and for $j = 2k$ even, define

$$B(j,d) = (j+1)\left(\frac{(j+2)d}{4(j+1)}\right)^{j}. \tag{5}$$

Thus Theorems 2.1 and 2.2 can be restated as $\det AA^{\mathrm{T}} \leqslant B(j,d)$ for all $A \in M_{j,d}(0,1)$ and $G(j,d) = B(j,d)$ whenever there exists a $j \times d$ regular D-optimal matrix.

It is easy to see from conditions 2b in Theorems 2.1 and 2.2 that a $j \times d$ regular D-optimal matrix exists only if

$$\begin{aligned} &2(j+1) \text{ divides } d \quad \text{for } j \equiv 0 \pmod 4,\\ &2j \text{ divides } d \quad \text{for } j \equiv 1 \pmod 4,\\ &j+1 \text{ divides } d \quad \text{for } j \equiv 2 \pmod 4,\\ &j \text{ divides } d \quad \text{for } j \equiv 3 \pmod 4. \end{aligned} \tag{6}$$

So unless the appropriate divisibility condition holds, $G(j,d) < B(j,d)$. For each j, $j \times d$ regular D-optimal matrices are known to exist for certain values of d. For $j = 2k - 1$ odd and $d = C(j,k)$ (the combinatorial coefficient), the $j \times d$ matrix whose columns consist of all (0,1)-j-tuples with exactly k ones is a regular D-optimal matrix [3]. For $j = 2k$ even and $d = C(j+1,k)$, the $j \times d$ matrix whose columns consist of all (0,1)-j-tuples with exactly k or $k+1$ ones is a regular D-optimal matrix [4]. These values of d are quite large compared to the smallest possible values for d that satisfy the necessary divisibility condition (6) for regular D-optimality. But in Section 3 we construct $j \times d$ regular D-optimal matrices for certain values of j with

$$\begin{aligned} &d = 2(j+1) \quad \text{for } j \equiv 0 \pmod 4, \\ &d = 2j \quad \text{for } j \equiv 1 \pmod 4, \\ &d = j+1 \quad \text{for } j \equiv 2 \pmod 4, \\ &d = j \quad \text{for } j \equiv 3 \pmod 4. \end{aligned} \tag{7}$$

We finish this section with two lemmas that describe ways to construct new regular D-optimal matrices from a given regular D-optimal matrix.

Lemma 2.1. *Let $j = 2k - 1$ be odd and let $A \in M_{j,d}(0,1)$ be a regular D-optimal matrix. Let $B \in M_{j-1,d}(0,1)$ be the matrix obtained by deleting any row from A. Then B is a regular D-optimal matrix.*

Proof. Suppose $A \in M_{j,d}(0,1)$ is a regular D-optimal matrix: $AA^{\mathrm{T}} = t(I_j + J_j)$, for some t and each column of A has exactly k ones. It is clear that $BB^{\mathrm{T}} = t(I_{j-1} + J_{j-1})$ and each column of B contains either k or $k+1$ ones. Thus B is a regular D-optimal matrix. □

Lemma 2.2. *Let $A \in M_{j,d}(0,1)$ be a regular D-optimal matrix and m be a positive integer. Then $m * A \in M_{j,md}(0,1)$ is a regular D-optimal matrix.*

Proof. $(m * A)(m * A)^{\mathrm{T}} = mAA^{\mathrm{T}}$. Thus if $AA^{\mathrm{T}} = t(I + J)$, then $(m * A)(m * A)^{\mathrm{T}} = mt(I + J)$. The result now follows since each column of $m * A$ is a column of A. □

3. D-optimal matrices arising from combinatorial designs

In this section regular D-optimal matrices are constructed for the values of d in Eq. (7). Although the construction is not possible for all j, we show that certain (v,k,λ)-designs can be used to construct regular D-optimal matrices. All of the necessary definitions and proofs about (v,k,λ)-designs are in [5], but we shall give a brief description and elementary properties here.

Definition 3.1. Let v, k, λ be positive integers with $k < v$. A (v, k, λ)-*design* is a finite collection $\mathscr{B} = \{B_1, \ldots, B_b\}$ of subsets of $\{1, 2, \ldots, v\}$ such that
1. each B_l has cardinality k, and
2. each pair $i, j \in \{1, \ldots, v\}$ occurs in exactly λ subsets in $\mathscr{B}$.

It is an elementary result in block design theory that if $\mathscr{B}$ is a (v, k, λ)-design, then each element $i \in \{1, \ldots, v\}$ occurs in the same number r of subsets in $\mathscr{B}$ and that b, r satisfy the conditions

$$\lambda(v-1) = r(k-1), \qquad bk = vr.$$

Thus b and r are determined by the other three parameters v, k, λ of the design. We shall refer to a (v, k, λ)-design as a (v, b, r, k, λ)-design. The general problem of determining whether a (v, b, r, k, λ)-design exists for given integers v, k, λ is unsolved. But infinite families of (v, b, r, k, λ)-designs have been constructed.

The object of interest to us is the *incidence matrix* $K = (k_{i,j})$ of a (v, b, r, k, λ)-design $\mathscr{B}$ defined by

$$k_{i,l} = \begin{cases} 1 & \text{if } i \in B_l, \\ 0 & \text{otherwise.} \end{cases}$$

(In most combinatorial books the incidence matrix is K^{T}.) The elementary properties of a (v, b, r, k, λ)-design are captured by the matrix equations

$$KK^{\mathrm{T}} = (r-\lambda)I_v + \lambda J_v, \tag{8}$$
$$J_v K = kJ_{v,b}.$$

In our notation for D-optimal matrices, $v = j$ and $b = d$. We will use j, d instead of v, b henceforth so that Eq. (8) becomes

$$KK^{\mathrm{T}} = (r-\lambda)I_j + \lambda J_j. \tag{9}$$

Eq. (9) resembles condition 1 for regular D-optimality in Theorem 2.1. In fact, for j odd, the incidence matrices for certain (v, b, r, k, λ)-designs lead to regular D-optimal matrices.

First we consider the case where $j = 4t - 1 \equiv 3 \pmod 4$. It is well known [5] that a $(4t-1, 4t-1, 2t-1, 2t-1, t-1)$-design exists if and only if a Hadamard matrix of order $4t$ exists. In fact the incidence matrix for a $(4t-1, 4t-1, 2t-1, 2t-1, t-1)$-design can be constructed directly from a $4t \times 4t$ Hadamard matrix. Let H be the incidence matrix for a $(4t-1, 4t-1, 2t-1, 2t-1, t-1)$-design. Specializing Eq. (9) we get

$$HH^{\mathrm{T}} = tI + (t-1)J.$$

H does not satisfy condition 1 for regular D-optimality in Theorem 2.1, but its complement $A = J - H$ does:

$$AA^{\mathrm{T}} = (J - H)(J - H)^{\mathrm{T}} = (4t - 1)J - 2(2t - 1)J + tI + (t - 1)J$$
$$= t(I + J).$$

And since $j = d = 4t - 1$, we have

$$\frac{(j + 1)d}{4j} = t.$$

Thus A is a regular D-optimal matrix. Combining this with Lemmas 2.1 and 2.2, we obtain the next theorem.

Theorem 3.1. *Let m be a positive integer, $j = 4t - 1$, $H \in M_{j,j}(0, 1)$ be the incidence matrix for a $(4t - 1, 4t - 1, 2t - 1, 2t - 1, t - 1)$-design, $A = J - H$, and let B be the matrix obtained by removing any row from A. Then $m * A$ and $m * B$ are regular D-optimal matrices.*

$(4t - 1, 4t - 1, 2t - 1, 2t - 1, t - 1)$-designs (sometimes known as Hadamard designs) are conjectured to exist for all integers $j \equiv 3 \pmod 4$ and the smallest integer for which the existence of a Hadamard design is in question is $j = 427$ (see [6]).

When $j \equiv 1 \pmod 4$ the situation changes. There are no $j \times j$ regular D-optimal matrices. (See (6).) But if $j = 4t + 1$ is a power of a prime, then a $j \times 2j$ regular D-optimal matrix *does* exist and can be constructed explicitly from a combinatorial object called a supplementary difference set in the Galois field GF(j) [5]. (Later, we give an example of this construction.) The construction produces a $(4t + 1, 8t + 2, 4t, 2t, 2t - 1)$-design. Let K be the incidence matrix for this design. Then from Eq. (9)

$$KK^{\mathrm{T}} = (2t + 1)I_j + (2t - 1)J_j,$$

and the matrix $A = J_{j,2j} - K$ satisfies condition 1 of Theorem 2.1.

$$AA^{\mathrm{T}} = J_{j,2j}J_{2j,j} - J_{j,2j}K^{\mathrm{T}} - KJ_{2j,j} + KK^{\mathrm{T}}$$
$$= 2(4t + 1)J_j - 4tJ_j - 4tJ_j + (2t + 1)I_j + (2t - 1)J_j$$
$$= (2t + 1)(I_j + J_j).$$

A also satisfies condition 2b of Theorem 2.1 since $(j + 1)/(4j) = 2t + 1$ and so A is a regular D-optimal matrix. Now using Lemmas 2.1 and 2.2 we obtain the following result.

Theorem 3.2. *Let m be a positive integer and $j = 4t + 1$ be a power of a prime. Let $K \in M_{j,2j}(0, 1)$ be the incidence matrix of a $(4t + 1, 8t + 2, 4t, 2t, 2t - 1)$-design, $A = J_{j,2j} - K$, and let $B \in M_{j-1,2j}$ be a matrix obtained by deleting any row of A. Then $m * A$ and $m * B$ are regular D-optimal matrices.*

More generally, if a supplementary difference set with parameter $\mathrm{SDS}(4t+1; 2t+1, 2t+1; 2t+1)$ exists in an abelian group G of order $4t+1$, then the concatenation of the incidence matrices provides a D-optimal $(4t+1) \times (8t+1)$ matrix. We omit the details. The smallest $j \equiv 1 \pmod 4$ for which we do not know a D-optimal matrix of size $j \times 2j$ is $j = 21$.

We conclude this section with a description of the construction of the 9×18 incidence matrix of a $(9, 18, 8, 4, 3)$-design.

Example 3.1. Let

$$\mathrm{GF}(9) = Z_3[x]/(x^2+1) = \{0, 1, \theta, \theta^2, \ldots, \theta^7\}$$

be the Galois field with 9 elements, where $\theta = x + 2$ generates the group of units in GF(9). We define two 9×9 matrices K_1, K_2 so that $K = [K_1, K_2]$ satisfies $KK^{\mathrm{T}} = 5I_9 + 3J_9$.

Let $Q = \{1, \theta^2, \theta^4, \theta^6\}$ consist of the quadratic residues of GF(9). Let $R = \{\theta, \theta^3, \theta^5, \theta^7\}$. The rows and columns of K_1 and of K_2 are indexed by the elements of GF(9) in this order: $0, 1, \theta, \theta^2, \ldots, \theta^7$. For $\alpha, \beta \in \mathrm{GF}(9)$,

$$(K_1)_{\alpha,\beta} = \begin{cases} 1 & \text{if } \beta \in \alpha + Q, \\ 0 & \text{otherwise.} \end{cases}$$

For example, if $\alpha = \theta^2$, then

$$\alpha + Q = \{\theta^2 + 1, \theta^2 + \theta^2, \theta^2 + \theta^4, \theta^2 + \theta^6\} = \{\theta^7, \theta^6, \theta, 0\}$$

So row θ^2 (the 4th row) of K_1 is $(1, 0, 1, 0, 0, 0, 0, 1, 1)$.

$$K_1 = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

To construct K_2, repeat the procedure used to construct K_1 but with R in place of Q. A direct calculation verifies that $[K_1, K_2][K_1, K_2]^{\mathrm{T}} = K_1K_1^{\mathrm{T}} + K_2K_2^{\mathrm{T}} = 5I_9 + 3J_9$.

4. Structure of D-optimal designs for large d

In this section we prove the statistically plausible result that for a given number of j objects and a sufficiently large number d of weighings, each weighing in a D-optimal design must contain about half of the objects.

Theorem 4.1. 1. *For $j = 2k - 1$ odd, there exists a positive integer d_0 such that for all $d \geqslant d_0$ each column of a D-optimal matrix $A \in M_{j,d}(0,1)$ has exactly k ones.*

2. *For $j = 2k$ even, there exists a positive integer d_0 such that for all $d \geqslant d_0$ each column of a D-optimal matrix $A \in M_{j,d}(0,1)$ has exactly k or $k+1$ ones.*

The proof of the theorem proceeds in three steps. In Lemma 4.1 we give an upper bound on $\det AA^{\mathrm{T}}$ for matrices A that contain a column with fewer than k or more than k ones (in the case $j = 2k - 1$) or fewer than k or more than $k + 1$ ones (in case $j = 2k$). Next we exhibit lower bounds for $G(j,d)$, the maximum of $\det AA^{\mathrm{T}}$ for $A \in M_{j,d}(0,1)$. This is done in Lemma 4.2. Finally the upper bounds on $\det AA^{\mathrm{T}}$ in Lemma 4.1 are shown to be less than the lower bounds on $G(j,d)$ in Lemma 4.2, for sufficiently large values of d. Hence $\det AA^{\mathrm{T}} < G(j,d)$ and A is not D-optimal.

Lemma 4.1. 1. *Assume that $j = 2k - 1$ and $A \in M_{j,d}(0,1)$ contains a column with fewer than k or more than k ones. Then*

$$\det AA^{\mathrm{T}} \leqslant \left(\frac{1}{j+1}\right)^{j-1} \left(\frac{k^2 d - 1}{j}\right)^{j}. \tag{10}$$

2. *Assume that $j = 2k$ and $A \in M_{j,d}(0,1)$ contains a column with fewer than k or more than $k + 1$ ones. Then*

$$\det AA^{\mathrm{T}} \leqslant \left(\frac{1}{j+1}\right)^{j-1} \left(\frac{k(k+1)d - 2}{j}\right)^{j}. \tag{11}$$

Proof. Assume that $j = 2k - 1$ and that $A \in M_{j,d}(0,1)$. Let n_r be the number of columns in A with r ones, $r = 1, \ldots, j$ and assume that $n_r \geqslant 1$ for some $r \neq k$. Following an argument in [4], we compute that

$$\operatorname{trace}[(j+1)I - J]AA^{\mathrm{T}} = \operatorname{trace} A^{\mathrm{T}}[(j+1)I - J]A \tag{12}$$

$$= \sum_{r=1}^{j} r(j + 1 - r)n_r. \tag{13}$$

The maximum value of $r(j + 1 - r)$ for $r = 1, \ldots, j$ is k^2 and occurs when $r = k$. For $r \neq k$, $r(j + 1 - r) < k^2$. Thus

$$\sum_{r=1}^{j} r(j+1-r)n_r < k^2 \sum_{r=1}^{j} n_r \tag{14}$$

$$= k^2 d. \tag{15}$$

So

$$\operatorname{trace}[(j+1)I - J]AA^{\mathrm{T}} \leqslant k^2 d - 1. \tag{16}$$

Applying the arithmetic-geometric-mean inequality to the eigenvalues of $[(j+1)I - J]AA^{\mathrm{T}}$ (which are nonnegative), we get

$$\det[(j+1)I - J]AA^{\mathrm{T}} \leqslant \left(\frac{k^2 d - 1}{j}\right)^{j}. \tag{17}$$

But $\det[(j+1)I - J] = (j+1)^{(j-1)}$ and hence

$$\det AA^{\mathrm{T}} \leqslant \left(\frac{1}{j+1}\right)^{j-1} \left(\frac{k^2 d - 1}{j}\right)^{j}. \tag{18}$$

The proof for the case $j = 2k$ is similar. $\square$

In Section 3 we saw that for each j, there is a c_0 and a $j \times c_0$ regular D-optimal matrix A_0. Thus, $G(j, c_0) = B(j, c_0)$. Also when $d = mc_0$ is a multiple of c_0, Lemma 2.2 guarantees a regular D-optimal matrix and again $G(j, mc_0) = B(j, mc_0)$. In the next lemma we use these matrices A_0 to obtain, for each j, d, a lower bound on $G(j, d)$, when d is not necessarily a multiple of c_0.

Lemma 4.2. *Let j be fixed and let c_0 be a positive integer such that there exists a regular D-optimal matrix $A_0 \in M_{j,c_0}(0,1)$. Then for all $d = tc_0 + m$, $1 \leqslant t$, $0 \leqslant m < c_0$, we have*

$$G(j,d) \geqslant \begin{cases} 2k\left(\frac{(j+1)c_0}{4j}\right)^{j} t^{j} + mk^2\left(\frac{(j+1)c_0}{4j}\right)^{j-1} t^{j-1} & \text{if } j = 2k-1, \\ (1+2k)\left(\frac{(j+2)c_0}{4(j+1)}\right)^{j} t^{j} + mk(k+1)\left(\frac{(j+2)c_0}{4(j+1)}\right)^{j-1} t^{j-1} & \text{if } j = 2k. \end{cases} \tag{19}$$

In particular, for $c_0 = C(j, k)$ (if j is odd) or $C(j+1, k)$ (if j is even),

$$G(j,d) \geqslant$$
$$\begin{cases} 2kC(2k-3, k-1)^{j} t^{j} + mk^2 C(2k-3, k-1)^{j-1} t^{j-1} & \text{if } j = 2k-1, \\ (1+2k)C(2k-1, k)^{j} t^{j} + mk(k+1)C(2k-1, k)^{j-1} t^{j-1} & \text{if } j = 2k. \end{cases} \tag{20}$$

Proof. First assume $j = 2k - 1$. Let $v^{\mathrm{T}} = (1, \ldots, 1, 0, \ldots, 0)$ have k ones. Let $A = [t * A_0, v, \ldots, v]$ with m copies of v adjoined to $t * A_0$. From Theorem 2.1 we have

$$A_0A_0^{\mathrm{T}} = \frac{(j+1)c_0}{4j}(I+J).$$

Thus,

$$\begin{aligned} AA^{\mathrm{T}} &= tA_0A_0^{\mathrm{T}} + \begin{pmatrix} mJ_k & 0 \\ 0 & 0 \end{pmatrix} = t\frac{(j+1)c_0}{4j}(I+J) + \begin{pmatrix} mJ_k & 0 \\ 0 & 0 \end{pmatrix} \\ &= xI + \begin{pmatrix} (x+m)J_k & xJ_{k,k-1} \\ xJ_{k-1,k} & xJ_{k-1} \end{pmatrix} = xI + R, \end{aligned}$$

where $x = t(j+1)c_0/4j$ and R is the rank 2 matrix. It is easy to see that trace $R = k(x+m) + (k-1)x = 2kx + mk - x$ and that the sum of all principal 2×2 minors of R is $k(k-1)mx$. Thus if λ_1 and λ_2 are the two nonzero eigenvalues of R, then $\lambda_1 + \lambda_2 = 2kx + mk - x$ and $\lambda_1\lambda_2 = k(k-1)mx$. Hence

$$\begin{aligned} \det AA^{\mathrm{T}} &= \det(xI+R) = (x+\lambda_1)(x+\lambda_2)x^{j-2} \\ &= x^j + (2kx + mk - x)x^{j-1} + k(k-1)mxx^{j-2} \\ &= 2kx^j + mk^2x^{j-1} = 2k\left(\frac{(j+1)c_0}{4j}\right)^j t^j + mk^2\left(\frac{(j+1)c_0}{4j}\right)^{j-1} t^{j-1}. \end{aligned}$$

The result now follows for $j = 2k - 1$.

Now if $j = 2k$, let $v^{\mathrm{T}} = (1, \ldots, 1, 0, \ldots, 0)$ have k ones and k zeros. Set $A = [t * A_0, v, \ldots, v]$. Then as above we have

$$\begin{aligned} AA^{\mathrm{T}} &= tA_0A_0^{\mathrm{T}} + \begin{pmatrix} mJ_k & 0 \\ 0 & 0 \end{pmatrix} = t\frac{(j+2)c_0}{4(j+1)}(I+J) + \begin{pmatrix} mJ_k & 0 \\ 0 & 0 \end{pmatrix} \\ &= xI + \begin{pmatrix} (x+m)J_k & xJ_k \\ xJ_k & xJ_k \end{pmatrix} = xI + R, \end{aligned}$$

where $x = t(j+2)c_0/4(j+1)$ and R is the rank 2 matrix. It is easy to see that trace $R = k(x+m) + kx = 2kx + mk$ and that the sum of all principal 2×2 minors of R is k^2mx. Thus if λ_1 and λ_2 are the two nonzero eigenvalues of R, then $\lambda_1 + \lambda_2 = 2kx + mk$ and $\lambda_1\lambda_2 = k^2mx$. Hence

$$\begin{aligned} \det AA^{\mathrm{T}} &= \det(xI+R) = (x+\lambda_1)(x+\lambda_2)x^{j-2} \\ &= x^j + (2kx + mk)x^{j-1} + k^2mxx^{j-2} = (1+2k)x^j + mk(k+1)x^{j-1} \\ &= (1+2k)\left(\frac{(j+2)c_0}{4(j+1)}\right)^j t^j + mk(k+1)\left(\frac{(j+2)c_0}{4(j+1)}\right)^{j-1} t^{j-1}. \end{aligned}$$

The result follows for $j = 2k$.

For $j = 2k - 1$ and $c_0 = C(j,k)$, there is a matrix $A_0 \in M_{j,c_0}(0,1)$ with $\det A_0A_0^{\mathrm{T}} = B(j, c_0)$. Replacing c_0 with $C(j,k)$ in Eq. (19) gives

$$\frac{(j+1)c_0}{4j} = C(2k-3, k-1),$$

which proves the first inequality of Eq. (20). The second inequality follows in the same way. For $j = 2k$ and $c_0 = C(j+1,k)$, there is a matrix $A_0 \in M_{j,c_0}(0,1)$ for which $\det A_0A_0^{\mathrm{T}} = B(j,c_0)$. It is easy to compute that

$$\frac{(j+2)c_0}{4(j+1)} = C(2k-1,k). \qquad \square$$

We could have improved the lower bound of the Lemma 4.2 by adjoining different vectors instead of multiple copies of v. However, we are interested only in the asymptotic result here.

The final step in the proof of Theorem 4.1 is to compare the bounds obtained in the previous two lemmas.

Proof of Theorem 4.1. Assume that $j = 2k-1$ and that $A \in M_{j,d}(0,1)$ is a D-optimal matrix. Also assume that some column of A does not have exactly k ones. Let $c_0 = C(j,k)$ and $d = tc_0 + m$, where $0 \leqslant m < c_0$. Let $f(t)$ be the lower bound for $G(j,d)$ in Eq. (20) of Lemma 4.2:

$$f(t) = 2kC(2k-3,k-1)^j t^j + mk^2C(2k-3,k-1)^{j-1}t^{j-1}$$

Let $g(t)$ be the upper bound on $\det AA^{\mathrm{T}}$ for matrices having a column with fewer than or more than k ones:

$$\begin{aligned} g(t) &= \left(\frac{1}{j+1}\right)^{j-1}\left(\frac{k^2d-1}{j}\right)^j = 2k\left(\frac{k^2C(j,k)t+k^2m-1}{(j+1)j}\right)^j \\ &= 2k\left(\frac{k^2C(j,k)}{(j+1)j}\right)^j t^j + 2kj\left(\frac{k^2C(j,k)}{(j+1)j}\right)^{j-1}\left(\frac{k^2m-1}{(j+1)j}\right)t^{j-1} + r(t) \\ &= 2kC(2k-3,k-1)^j t^j + mk^2C(2k-3,k-1)^{j-1}t^{j-1} \\ &\quad - C(2k-3,k-1)^{j-1}t^{j-1} + r(t), \end{aligned}$$

where $r(t)$ is a polynomial of degree $\leqslant j-2$ in t. Then

$$f(t) \leqslant \det AA^{\mathrm{T}} = G(j,d) \leqslant g(t). \tag{21}$$

Now consider

$$f(t) - g(t) = C(2k-3,k-1)^{j-1}t^{j-1} - r(t).$$

Since the degree of $r(t)$ is less than or equal to $j-2$, $f(t) > g(t)$ for sufficiently large values of t. That is, there exists t_0 such that $f(t) > g(t)$ for all $t > t_0$, which contradicts the D-optimality of A. It follows that if $A \in M_{j,d}(0,1)$ is a D-optimal matrix and $d > c_0t_0$, then all columns of A must contain exactly k ones. Thus the first part ($j = 2k-1$ odd) of Theorem 4.1 is proved.

The analysis for $j = 2k$ is analogous to the one for $j = 2k-1$. Again, suppose that $A \in M_{j,d}(0,1)$ is a D-optimal matrix and that some column of A has fewer than k ones or more than $k+1$ ones. Set $c_0 = C(j+1,k)$. As above, let

$f(t)$ be the lower bound on $G(j,d)$ from Lemma 4.2 and let $g(t)$ be the upper bound on $\det AA^{\mathrm{T}}$ from Lemma 4.1, i.e.

$$\begin{aligned} f(t) &= (2k+1)C(2k-1,k)^j t^j + mk(k+1)C(2k-1,k)^{j-1}t^{j-1} \\ g(t) &= (2k+1)\left(\frac{k(k+1)C(2k+1,k)t+mk(k+1)-2}{j(j+1)}\right)^j \\ &= (2k+1)\left(\frac{k(k+1)C(2k+1,k)}{(j+1)j}\right)^j t^j \\ &\quad + (2k+1)\left(\frac{k(k+1)C(2k+1,k)}{(j+1)j}\right)^{j-1}\left(\frac{k(k+1)m-2}{j+1}\right)t^{j-1}+r(t) \\ &= (2k+1)C(2k-1,k)^j t^j + mk(k+1)C(2k-1,k)^{j-1}t^{j-1} \\ &\quad - 2C(2k-1,k)^{j-1}t^{j-1}+r(t), \end{aligned}$$

where $r(t)$ is a polynomial of degree $\leqslant j-2$ in t. Hence

$$f(t)-g(t) = 2C(2k-1,k)t^{j-1}-r(t). \tag{22}$$

Thus there exists a t_0 such that for all $t \geqslant t_0$ $f(t)-g(t)>0$, a contradiction to the D-optimality of A. Thus, if $d_0 = t_0c_0$ and $d \geqslant d_0$, then all columns of a D-optimal $(0,1)$ matrix of size $j \times d$ have either k or $k+1$ ones. □

5. The connection with (± 1) D-optimal designs

Let A be a $j \times j$ (0,1)-matrix and let B be the $(j+1)\times(j+1)$ (± 1)-matrix defined by

$$B = \begin{pmatrix} 1 & J_{1,j} \\ J_{j,1} & J_j - 2A \end{pmatrix}.$$

It is easy to show that $|\det B| = 2^j|\det A|$. This well-known connection makes the problem of finding matrices in $M_{j,j}(0,1)$ with determinant of maximum absolute value equivalent to the problem of finding matrices in $M_{j+1,j+1}(\pm 1)$ with determinant of maximum absolute value. In this section we develop an analogous connection between (0,1)- and (± 1)-matrices that are *not* square and use it to show that certain (0,1)-matrices are D-optimal. In fact, we exhibit infinite families of *nonregular* D-optimal matrices. Throughout, we assume that $j = 2k-1$ is odd. As we shall see, our methods do not work for j even.

Lemma 5.1. *Let $j = 2k-1, p \geqslant 0$ and let $A \in M_{j,d}(0,1)$ have exactly k ones in each of its columns. Define a matrix $L(A) \in M_{j+1,d+p}(\pm 1)$ by*

$$L(A) = \left[\begin{array}{c|c} J_{1,d} & J_{1,p} \\ \hline J_{j,d}-2A & J_{j,p} \end{array}\right].$$

Then $\det L(A)L(A)^{\mathrm{T}} = p\,4^j \det AA^{\mathrm{T}}$.

Proof. Perform the following elementary row operations on $L(A)$:
Subtract row 1 from all other rows of $L(A)$ to get

$$L_1(A) = \left[\begin{array}{c|c} J_{1,d} & J_{1,p} \\ \hline -2A & 0_{j,p} \end{array}\right].$$

Add $1/2k$ times rows 2 through $j+1$ to row 1 of $L_1(A)$ to get

$$L_2(A) = \left[\begin{array}{c|c} 0_{1,d} & J_{1,p} \\ \hline -2A & 0_{j,p} \end{array}\right].$$

Since $\det L(A)L(A)^{\mathrm{T}} = \det L_2(A)L_2(A)^{\mathrm{T}}$ the result follows. □

Now fix $j = 2k - 1$ and suppose d is large enough to insure (by Theorem 4.1) that each column of a D-optimal matrix in $M_{j,d}(0,1)$ has exactly k ones. Further, suppose $A \in M_{j,d}(0,1)$, A has exactly k ones in each column, and $L(A)$ is a D-optimal matrix in $M_{j+p,d+1}(\pm 1)$. Then A must be D-optimal. To see this, suppose that $A_0 \in M_{j,d}(0,1)$ is D-optimal. By Theorem 4.1, A_0 has exactly k ones in each column. Now $\det L(A_0)L(A_0)^{\mathrm{T}} \leqslant \det L(A)L(A)^{\mathrm{T}}$ since $L(A)$ is D-optimal. Then from Lemma 5.1, $\det A_0A_0^{\mathrm{T}} \leqslant \det AA^{\mathrm{T}}$. But since A_0 is D-optimal, $\det A_0A_0^{\mathrm{T}} = \det AA^{\mathrm{T}}$ and so A is also D-optimal. We shall use this observation (in Theorem 5.2) to prove that certain matrices $A \in M_{j,d}(0,1)$ are D-optimal by showing that $L(A) \in M_{j+1,d+p}(\pm 1)$ is D-optimal.

Unfortunately the same argument cannot be used for $j = 2k$ even. Indeed, if d is sufficiently large and $A_0 \in M_{j,d}(0,1)$ is D-optimal, then some of the columns of A_0 can have k ones while other columns have $k+1$ ones. In that case the upper left block of $L_2(A)$ from Lemma 5.1 will not consist of zeros. Apparently the only way to produce a (± 1)-matrix $L(A)$ from a (0,1)-matrix A so that the determinants of the two matrices are related in a reasonable way is for each column of A to have the same number of ones.

In the next theorem we summarize known results for D-optimality of (± 1)-matrices. Then in Theorem 5.2 these results are used to prove that certain families of (0,1)-matrices are D-optimal.

Theorem 5.1. *Assume that* $B \in M_{j,d}(\pm 1)$.
1. ([7]) *If* $d \equiv 0 \pmod 4$ *and* $BB^{\mathrm{T}} = dI_j$, *then B is D-optimal. In particular,* $\det BB^{\mathrm{T}} \leqslant d^j$ *for all* $B \in M_{j,d}(\pm 1)$.
2. ([8–10]) *If* $d \equiv 1 \pmod 4$ *and* $BB^{\mathrm{T}} = (d-1)I_j + J_j$, *then B is D-optimal. In particular,* $\det BB^{\mathrm{T}} \leqslant (d-1)^{j-1}(d+j-1)$ *for all* $B \in M_{j,d}(\pm 1)$.
3. ([12,9,11]) *If* $d \equiv 2 \pmod 4$ *and*

$$BB^{\mathrm{T}} = \begin{cases} \begin{pmatrix} (d-2)I_k + 2J_k & 0 \\ 0 & (d-2)I_k + 2J_k \end{pmatrix} & \textit{if } j = 2k, \\ \begin{pmatrix} (d-2)I_k + 2J_k & 0 \\ 0 & (d-2)I_{k-1} + 2J_{k-1} \end{pmatrix} & \textit{if } j = 2k-1, \end{cases}$$

then B is D-optimal. In particular, $\det BB^{\mathrm{T}} \leqslant (d-2)^{j-2}(d+j-2)^2$ *if j is even and* $\det BB^{\mathrm{T}} \leqslant (d-2)^2(d+j-3)^{(t-3)/2}(d+j-1)^{(t-1)/2}$, *if j is odd.*

4. ([13,14]) *If $2j-5 \leqslant d \equiv 3 \pmod 4$ and $BB^{\mathrm{T}} = (d+1)I_j - J_j$, then B is D-optimal. In particular,* $\det BB^{\mathrm{T}} \leqslant (d+1)^{j-1}(d-j+1)$, *for all $B \in M_{j,d}(\pm 1)$.*

Of course, if $B \in M_{j,d}(\pm 1)$ and BB^{T} is similar to one of the D-optimal matrices in Theorem 5.1, then B is also D-optimal.

The main result of this section produces new infinite families of D-optimal matrices. Some of them were conjectured to be D-optimal in [3].

Theorem 5.2. *Let $j = 2k-1$ be odd and let d_0 be the constant of Theorem* 4.1. *Let $A_0 \in M_{j,d}(0,1)$, $d \geqslant d_0$, be a regular D-optimal matrix.*

1. *Let $A_1 = [A_0, v]$ where $v^{\mathrm{T}} = (0,\dots,0,1,\dots,1)$ has k ones. Then A_1 is D-optimal.*
2. *Assume $j < d$. Let A_1 be obtained from A_0 be deleting a column of A_0. Then A_1 is D-optimal.*
3. *Assume that $j = 4k-1 \equiv 3 \pmod 4$. Let $A_1 = [A_0, v_1, v_2]$ where*

$$\begin{aligned} v_1^{\mathrm{T}} &= (0,\dots,0 \quad 0,\dots,0 \quad 1,\dots,1 \quad 1,\dots,1) \\ v_2^{\mathrm{T}} &= (\underbrace{0,\dots,0}_{k-1} \quad \underbrace{1,\dots,1}_{k} \quad \underbrace{0,\dots,0}_{k} \quad \underbrace{1,\dots,1}_{k}). \end{aligned}$$

Then A_1 is D-optimal.

Proof. Suppose $A_0 \in M_{j,d}(0,1)$ and

$$\det A_0A_0^{\mathrm{T}} = B(j,d) = (j+1)\left(\frac{j+1}{j}\right)^j\left(\frac{d}{4}\right)^j.$$

From Theorem 2.1, we have $A_0A_0^{\mathrm{T}} = t(I_j + J_j)$, where $t = (j+1)d/4j$ is an integer. Consequently, $d/j = p$ is an integer and $d + p = 4t \equiv 0 \pmod 4$. By a direct calculation using $A_0A_0^{\mathrm{T}} = t(I_j + J_j)$, we see that $L(A_0)L(A_0)^{\mathrm{T}} = (d+p)I_{j+1}$.

1. Let $A_1 = [A_0, v] \in M_{j,d+1}(0,1)$ where $v^{\mathrm{T}} = (0,\dots,0,1,\dots,1)$. Then $L(A_1) \in M_{j+1,d+1+p}(\pm 1)$. Since A_1 has one more column than A_0, $L(A_1)$ has one more column than $L(A_0)$, namely $(1,\dots,1,-1,\dots,-1)$; this extra column has k ones and k negative ones. Thus

$$L(A_1)L(A_1)^{\mathrm{T}} = L(A_0)L(A_0)^{\mathrm{T}} + \begin{bmatrix} J_k & -J_k \\ -J_k & J_k \end{bmatrix} = (d+p)I_{j+1} + \begin{bmatrix} J_k & -J_k \\ -J_k & J_k \end{bmatrix}.$$

Since $d+1+p \equiv 1 \pmod 4$, we can use part 2 of Theorem 5.1. It is easy to see that $L(A_1)L(A_1)^{\mathrm{T}}$ is similar to $(d+p)I_{j+1}+J_{j+1}$ via the diagonal (± 1)-matrix $I_k \oplus (-I_k)$. Thus $L(A_1)$ is D-optimal, which implies that A_1 is D-optimal.

2. Without loss of generality, we may assume that the column deleted from A_0 is $v=(0,\ldots,0,1,\ldots,1)^{\mathrm{T}}$. By the definition of $A_1 \in M_{j+1,d+p-1}(0,1)$ and the same argument from part 1, we get

$$L(A_1)L(A_1)^{\mathrm{T}} + \begin{bmatrix} J_k & -J_k \\ -J_k & J_k \end{bmatrix} = L(A_0)L(A_0)^{\mathrm{T}}.$$

Thus,

$$L(A_1)L(A_1)^{\mathrm{T}} = (d+p)I_{j+1} - \begin{bmatrix} J_k & -J_k \\ -J_k & J_k \end{bmatrix}.$$

Now $d+p-1 \equiv 3 \pmod 4$. And since $j<d$ and $j|d$, we have $2j \leqslant d$. Thus $2(j+1)-5 \leqslant d-3 \leqslant d+p-1$ and so all of the conditions for part 4 of Theorem 5.1 are met. It follows that $L(A_1)$ is D-optimal. Hence A_1 is D-optimal.

3. By the definition of $A_1 \in M_{j+1,d+p+2}(0,1)$,

$$L(A_1)L(A_1)^{\mathrm{T}} = (d+p)I_{j+1} + \begin{bmatrix} 2J_k & 0 & 0 & -2J_k \\ 0 & 2J_k & -2J_k & 0 \\ 0 & -2J_k & 2J_k & 0 \\ -2J_k & 0 & 0 & 2J_k \end{bmatrix},$$

which is similar (by a permutation matrix and a diagonal ± 1 matrix) to

$$(d+p)I_{j+1} + \begin{bmatrix} 2J_k & 2J_k & 0 & 0 \\ 2J_k & 2J_k & 0 & 0 \\ 0 & 0 & 2J_k & 2J_k \\ 0 & 0 & 2J_k & 2J_k \end{bmatrix}.$$

Now $d+p+2 \equiv 2 \pmod 4$. Hence $L(A_1)$ is D-optimal by part 3 of Theorem 5.1. It follows that A_1 is D-optimal. □

To put things in perspective, we compare the results from Sections 2 and 3 with Theorem 5.2. For each j, there is a c_0 such that $j \times mc_0$ regular D-optimal matrices exist for all m. And for certain j, c_0 can be small; $c_0 = j$ (Theorem 3.1) or $c_0 = 2j$ (Theorem 3.2). Thus the question of determining $G(j, mc_0)$ is settled; $G(j, mc_0) = B(j, mc_0)$. But Theorem 5.2 settles the question for $d = mc_0 + r$, where $r = \pm 1, 2$, and m sufficiently large. In the next section we obtain weaker results for other values of r.

6. Nearly D-optimal matrices arising from Hadamard designs

Throughout this section we assume that $j = 4k - 1$ and that $A_0 \in M_{j,j}(0,1)$ is the complement of the incidence matrix of a $(4k-1, 4k-1, 2k-1, 2k-1, k-1)$-design (Hadamard design) so that

$$A_0 A_0^{\mathrm{T}} = \frac{j+1}{4}(I_j + J_j). \tag{23}$$

Following [3], Section 7, we construct a $j \times d$ (0,1)-matrix A, where $d = tj + r$, with $0 \leqslant r < j$ as follows.

$$A = [t * A_0, A_r], \tag{24}$$

where $A_r \in M_{j,r}(0,1)$ consists of the first r columns of A_0. For $j = 7$, A is conjectured [3], Section 6 to be D-optimal. In any case, det AA^{T} is a lower bound on the maximum value $G(j,d)$ of det XX^{T}, for $X \in M_{j,d}(0,1)$, which when compared to the upper bound given in Theorem 2.1 provides a tight estimate of $G(j,d)$. To be precise, define

$$L_{j,r}(t) = \det AA^{\mathrm{T}}.$$

The value of $L_{j,r}(t)$ is given in the next lemma.

Lemma 6.1 ([3], Theorem 7.1).

$$L_{j,r}(t) = 4\left(\frac{j+1}{4}\right)^{j+1}(t+1)^r t^{j-r}.$$

We compare this lower bound on $G(j,d)$ with the upper bound from Theorem 2.1 given by

$$U_{j,r}(t) = 4\left(\frac{j+1}{4}\right)^{j+1}\left(t + \frac{r}{j}\right)^j.$$

Thus,

$$L_{j,r}(t) \leqslant G(j,d) \leqslant U_{j,r}(t).$$

As polynomials in t, both $L_{j,r}(t)$ and $U_{j,r}(t)$ are of degree j. Furthermore, they agree in the first two terms of their expansions, viz.,

$$(t+1)^r t^{j-r} = t^j + rt^{j-1} + \frac{r(r-1)}{2}t^{j-2} + \cdots$$

$$\left(t + \frac{r}{j}\right)^j = t^j + rt^{j-1} + \frac{r^2(j-1)}{2j}t^{j-2} + \cdots$$

Next we present a short proof of the Lemma 6.1.

Proof. From Eq. (24), we have

$$AA^{\mathrm{T}} = tA_0A_0^{\mathrm{T}} + A_rA_r^{\mathrm{T}} = (A_0A_0^{\mathrm{T}})(tI_j + (A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}).$$

Since $A_0A_0^{\mathrm{T}} = ((j+1)/4)(I_j + J_j)$, $\det A_0A_0^{\mathrm{T}} = ((j+1)/4)^j(j+1)$. It remains to prove that

$$\det(tI_j + (A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}) = (t+1)^r t^{j-r}. \tag{25}$$

The nonzero eigenvalues of the $j \times j$ matrix $(A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}$ are the same as the eigenvalues of $A_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}A_r$. But $A_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}A_r$ is the $r \times r$ submatrix in the upper left corner of $A_0^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}A_0 = A_0^{\mathrm{T}}(A_0^{\mathrm{T}})^{-1}A_0^{-1}A_0 = I_j$. ($A_0$ is invertible.) Hence $A_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}A_r = I_r$. It follows that the eigenvalues of $(A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}$ are 1 (with multiplicity r and 0 (with multiplicity $j - r$). This establishes Eq. (25). □

We close this section with additional evidence that A defined in Eq. (24) may be D-optimal.

Theorem 6.1. *Let $j = 4k - 1$ and A_0 be the complement of the incidence matrix for a $j \times j$ $(4k-1, 4k-1, 2k-1, 2k-1, k-1)$-(Hadamard) design. Let $A = [t * A_0, A_r]$, where $0 \leqslant r < j$ and $A_r \in M_{j,r}(0,1)$ consists of the first r columns of A_0 and let $B = [t * A_0, B_r]$, where B_r is any $j \times r$ (0,1)-matrix. Then*

$$\det BB^{\mathrm{T}} \leqslant \det AA^{\mathrm{T}}, \tag{26}$$

with equality if and only if

$$B_r^{\mathrm{T}}B_r = \frac{j+1}{4}(I_r + J_r).$$

Proof. From the definitions of A and B, we have

$$BB^{\mathrm{T}} = tA_0A_0^{\mathrm{T}} + B_rB_r^{\mathrm{T}},$$
$$AA^{\mathrm{T}} = tA_0A_0^{\mathrm{T}} + A_rA_r^{\mathrm{T}}.$$

Thus

$$(A_0A_0^{\mathrm{T}})^{-1}BB^{\mathrm{T}} = tI_j + (A_0A_0^{\mathrm{T}})^{-1}B_rB_r^{\mathrm{T}}$$
$$(A_0A_0^{\mathrm{T}})^{-1}AA^{\mathrm{T}} = tI_j + (A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}},$$

and it suffices to show that

$$\det(tI_j + (A_0A_0^{\mathrm{T}})^{-1}B_rB_r^{\mathrm{T}}) \leqslant (t+1)^r t^{j-r} \tag{27}$$

$$= \det(tI_j + (A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}). \tag{28}$$

From Eq. (23), we have

$$(A_0A_0^{\mathrm{T}})^{-1} = \left(\frac{4}{j+1}\right)\left(I_j - \frac{1}{j+1}J_j\right).$$

Next consider

$$B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r = \frac{4}{j+1}B_r^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)B_r.$$

If the ith column v of B_r has s ones, then

$$v^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)v = s - \frac{s^2}{j+1} \tag{29}$$

$$\leqslant \frac{j+1}{4}, \tag{30}$$

with equality if and only if $s = (j+1)/2$. So the (i,i) entry of $B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r$ satisfies

$$(B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r)_{i,i} \leqslant 1,$$

for $i = 1, \dots, r$. Let $\lambda_1, \dots, \lambda_r$ be the (nonnegative) eigenvalues of $B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r$. Then

$$\tau = \sum \lambda_i = \mathrm{trace}(B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r) \leqslant r$$

and

$$\prod(t+\lambda_i) \leqslant \left(t + \frac{\tau}{r}\right)^r \leqslant (t+1)^r.$$

The eigenvalues of $(A_0A_0^{\mathrm{T}})^{-1}B_rB_r^{\mathrm{T}}$ are $\lambda_1, \dots, \lambda_r$, and 0 with multiplicity $j-r$. Thus

$$\begin{aligned}\det(tI_j + (A_0A_0^{\mathrm{T}})^{-1}B_rB_r^{\mathrm{T}}) &= t^{j-r}\prod(t+\lambda_i)\\ &\leqslant t^{j-r}\left(t+\frac{\tau}{r}\right)^r \leqslant t^{j-r}(t+1)^r\\ &= \det(tI_j + (A_0A_0^{\mathrm{T}})^{-1}A_rA_r^{\mathrm{T}}).\end{aligned}$$

Inequality Eq. (28) is proved.

Equality holds in Eq. (28) if and only if $\lambda_i = 1$ for $i = 1, \dots, r$, which holds if and only if $B_r^{\mathrm{T}}(A_0A_0^{\mathrm{T}})^{-1}B_r = I_r$. Suppose $B_r^{\mathrm{T}}B_r = ((j+1)/4)(I_r + J_r)$. Then each column of B_r has $(j+1)/2$ ones. And if u, v are different columns of B_r, then $u^{\mathrm{T}}v = (j+1)/4$. Thus

$$u^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)u = \frac{j+1}{4}$$

and

$$u^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)v = 0.$$

That is,

$$B_r^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)B_r = \frac{j+1}{4}I_r,$$

which is equivalent to $B_r(A_0A_0^{\mathrm{T}})^{-1}B_r = I_r$.

Conversely, suppose

$$B_r^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)B_r = \frac{j+1}{4}I_r$$

and that u, v are different columns of B_r. Since equality holds in Eq. (30), each column of B_r has $(j+1)/2$ ones. But

$$0 = u^{\mathrm{T}}\left(I_j - \frac{1}{j+1}J_j\right)v = u^{\mathrm{T}}v - \frac{1}{j+1}\left(\frac{j+1}{2}\right)^2 = u^{\mathrm{T}}v - \frac{j+1}{4}.$$

Thus $u^{\mathrm{T}}v = (j+1)/4$. It follows that $B_r^{\mathrm{T}}B_r = (j+1/4)(I_r + J_r)$. $\square$

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